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Extracting Physics from an Unphysical Situation: Light Mesons in a Small Box

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Quantum Chromo Dynamics is considered in a setup where the light mesons are squeezed into unphysically small boxes. We show how such a situation can be used to determine the couplings of the low energy chiral Lagrangian from lattice simulations, applying chirally invariant formulations of lattice fermions.

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1 Introduction

A straightforward approach for numerical simulations in statistical mechanics or in high energy physics is to perform them in boxes that are large enough for the relevant correlation lengths — or the Compton wave lengths of the lightest particles — to live comfortably inside the box. This is an ideal world and, as it might have been suspected, as far as numerical simulations are concerned this world is also very expensive. Approaching the critical point of a second order phase transition, where also a *continuum* field theory is defined, one needs to increase the correlation length, accompanied by the corresponding extension of the box size. For models in high energy physics the number of lattice points needed in the simulations has to be increased with the fourth power in this limit, and this does not even include additional factors originating from the scaling behavior of the algorithms employed.

It is one of the fascinating discoveries that physical models of interest can be considered in *unphysical* situations while it is still possible to extract correct physical information from it. The reason is that characteristic properties of a model do not change when it is considered under unphysical conditions. The advantage of this idea is that often the model can be considered in a setup where numerical simulations are much easier than in the case of a large physical volume.

Let us give a — not too serious — example to illustrate this idea: think of a folding chair. If it is unfolded (its physical state), you recognize it easily as a chair and you can use it as such. However, it would not fit into your car. Folding it (the unphysical state), you can put it in the car, but it is not recognizable easily as a chair anymore. Still, it is a chair, of course, and by measuring the length of the struts etc. (which do not change in the folded state) you can deduce the size of the original chair.

The idea of studying a system as a function of the box size in order to extract physical information is quite old and proved to be very fruitful. Finite size scaling arguments were already introduced 1883 by Reynolds for turbulence studies in air and liquid flows. Later on, they were applied in investigations of critical phenomena at phase transitions to extract critical exponents¹, to determine scattering lengths² and to renormalize scale dependent quantities such as the running strong coupling constant, the running quark masses and so-called renormalization constants^{3,4}. The physical problem we want to consider in the present article is the dynamics of Goldstone bosons as they appear in the case of a spontaneously broken continuous symmetry, such as the $O(N)$ symmetry in non-linear σ -models and the chiral symmetry in Quantum Chromo Dynamics (QCD) with massless quarks.

The dynamics of these Goldstone bosons can be described by *chiral perturbation theory*⁵, which evaluates the chiral Lagrangian. This Lagrangian describes the low energy properties of some underlying, more fundamental theory. It is constructed such that it obeys the same (global) symmetries as the fundamental theory. Examples are effective descriptions of the Φ^4 -theory and, of course, QCD for which chiral perturbation theory was designed. The structure of the chiral Lagrangian is very general. In leading order it can be written as

$$\mathcal{L}_{\text{eff}}[U] = \frac{F_\pi^2}{4} \text{Tr} \left[\partial_\mu U \partial_\mu U^\dagger \right] - \frac{1}{2} \Sigma m_q \text{Tr} \left[U e^{i\theta/N_f} + U^\dagger e^{-i\theta/N_f} \right]. \quad (1)$$

Here $U(x) \in SU(N_f)$ represents the Goldstone boson field, N_f is the number of flavors, m_q is the quark mass^a and θ is the vacuum angle. The Lagrangian in eq. (1) contains two so-called low energy constants (LEC), the *pion decay constant* F_π and the order parameter of chiral symmetry breaking, i.e. the *scalar condensate* Σ . Chiral perturbation theory allows for a systematic higher order expansion with more complicated terms in the Lagrangian and corresponding additional LEC multiplying these terms. The LEC are free parameters of the Lagrangian. They can only be determined by the comparison with sources beyond chiral perturbation theory. In principle, their values follow from the underlying fundamental theory, in this case QCD.

In the infinite volume (the standard regime of chiral perturbation theory) the Goldstone field U is parameterized as $U(x) = \exp \{ i\sqrt{2}\xi(x)/F_\pi \}$ with a fluctuating field $\xi(x)$. When the volume is taken to be small, the Compton wavelength of the Goldstone boson exceeds the finite physical extent L of the box. In this situation, the so-called ϵ -regime^{6,7}, the constant mode U_0 is separated and the field is written as $U(x) = U_0 \exp \{ i\sqrt{2}\tilde{\xi}(x)/F_\pi \}$ with $\int_V \tilde{\xi}(x) dx = 0$. The contribution of the constant mode U_0 to the chiral Lagrangian must be treated non-perturbatively.

The situation is illustrated in Figure 1 for the p -expansion and in Figure 2 for the ϵ -expansion. In the p -expansion regime, the pion Compton wavelength fits into the finite

^aFor simplicity we assume the same quark mass for all flavors. In a spin model it corresponds to an external magnetic field. Strictly speaking, due to $V < \infty$ and $m_q > 0$ this kind of symmetry breaking is not fully spontaneous and we actually deal with remnants of the Goldstone bosons.

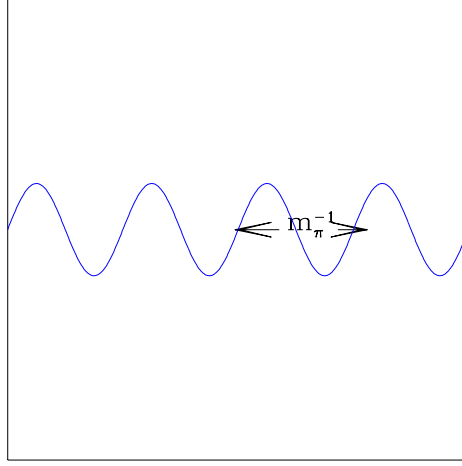


Figure 1. Illustration of the p -expansion regime. The Compton wavelength of the pion fits into the finite box.

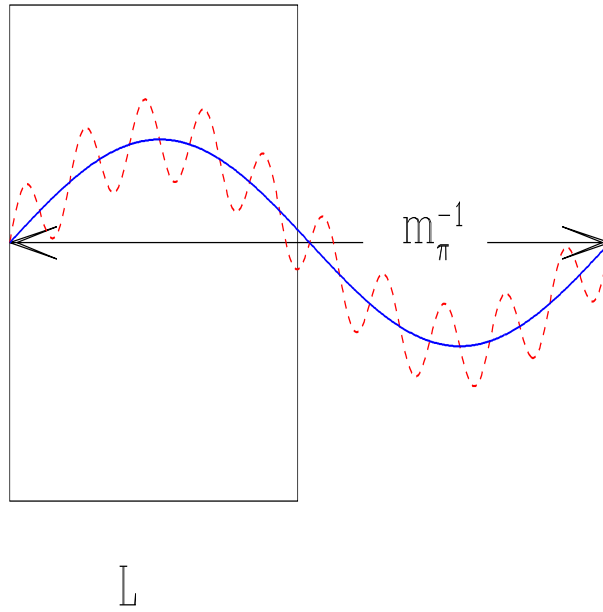


Figure 2. Illustration of the ϵ -regime. The Compton wavelength (blue solid line) exceeds the length of the box, whereas the fluctuations (red dashed line) do fit into the box.

box, corresponding to an infinite volume situation. In the ϵ -regime, the pion Compton wavelength exceeds the box length and the zero momentum pion mode appears as a con-

stant mode. Notice, however, that the fluctuations around the constant mode are still well accommodated within the box.

Numerical simulations are a powerful tool to determine the LEC. These simulations use the fundamental Lagrangian of QCD itself. Tuning the quark masses such that the regime of chiral perturbation theory is reached, a comparison of numerically generated QCD data and the predictions of chiral perturbation theory can be performed. In this way the LEC can be extracted by a fit of the numerical data to the analytical formulae of chiral perturbation theory, which contain the LEC as free parameters. The so determined values of the LEC as originating from QCD can then be related to experimental data leading to direct tests of QCD. In addition, the simulations can — in principle — be performed exploring different scenarios. For example one of the quark masses can be put to zero⁸ and it can be tested whether such a scenario would be consistent with the real world.

Knowing the LEC is also an important ingredient to supplement further numerical simulations themselves. Simulations at small values of the quark mass, corresponding to their physical values, are very expensive, see e.g. Ref. 9. If we would know, however, at what values of the quark mass chiral perturbation theory is valid, chiral perturbation theory itself could be used to extrapolate many observables to physical values of the quark mass. Obviously, for this procedure the knowledge of the LEC would be crucial.

Now the obvious question arises why such comparisons of simulation results and chiral perturbation theory have not been done before. The answer is, *they have*, but the interpretation of the outcome has been difficult and no convincing picture emerged. For the infinite volume simulations it is still not clear when contact to chiral perturbation theory can be established. Various additional assumptions have to be incorporated to the analytical computations in chiral perturbation theory to be able to relate them to numerical results¹⁰.

The finite volume simulations, which seem to be much easier, were hampered by the fact that the lattice formulations of fermion actions either break chiral symmetry explicitly (Wilson fermions) or that topological sectors are hard to distinguish (staggered fermions)¹¹. The identification of topological charge sectors is a necessary prerequisite for exploring the ϵ -regime, since here the observables depend strongly on the topology¹². Similar problems are encountered for improved versions of these lattice fermions.

A great leap forward was achieved with the rediscovery¹³ of the Ginsparg and Wilson¹⁴ relation which reads for some (yet to be specified) lattice Dirac operator D at $m_q = 0$

$$\gamma_5 D + D \gamma_5 = a D \gamma_5 D . \quad (2)$$

Clearly, in the limit of a vanishing lattice spacing a the usual anti-commutation relation of the continuum Dirac operator is recovered. The Ginsparg-Wilson relation implies an exact lattice chiral symmetry¹⁵ if the action is constructed with a lattice Dirac operator that solves the Ginsparg-Wilson relation. Consequently Ginsparg-Wilson fermions have a well defined fermionic index. By means of the Index Theorem, this property also allows for a conceptually clean separation of topological sectors¹³. Thus one overcomes the obstacles that other formulations of lattice fermions are plagued with.

For completeness we give a particular example for a solution of the Ginsparg-Wilson relation found by H. Neuberger¹⁶ from the overlap formalism¹⁷, based on the pioneering work by D. Kaplan¹⁸. To this end, we first consider the standard Wilson-Dirac operator on

the lattice,

$$D_w = \frac{1}{2} \{ \gamma_\mu (\nabla_\mu^* + \nabla_\mu) - a \nabla_\mu^* \nabla_\mu \} , \quad (3)$$

with ∇_μ , ∇_μ^* the lattice forward resp. backward derivatives, i.e. nearest neighbor differences acting on a field $\Phi(x)$,

$$\begin{aligned} \nabla_\mu \Phi(x) &= \frac{1}{a} [U(x, \mu) \Phi(x + a\hat{\mu}) - \Phi(x)] , \\ \nabla_\mu^* \Phi(x) &= \frac{1}{a} [\Phi(x) - U(x - a\hat{\mu}, \mu)^\dagger \Phi(x - a\hat{\mu})] . \end{aligned} \quad (4)$$

Here $U(x, \mu)$ is the link variable pointing from site x into the direction μ , and $\hat{\mu}$ is a unit vector in the same direction. We then define

$$A = D_w - 1 - s , \quad (5)$$

where the parameter s can be tuned in some interval. At last Neuberger's overlap operator D_N with mass m is given by

$$\begin{aligned} D_N &= \left\{ 1 - \frac{m_q}{2(1+s)} D_N^{(0)} \right\} + m_q , \\ D_N^{(0)} &= (1+s) \left[1 + A(A^\dagger A)^{-1/2} \right] . \end{aligned} \quad (6)$$

Despite the appearance of the square root which connects all the lattice point with each other, the operator is local (in the field theoretical sense) as long as the gauge coupling is not too strong¹⁹. However, the numerical implementation of the square root operator is very demanding and restricts present simulation to the quenched approximation^b, see also the reviews^{20,21}. A promising approach for a construction of improved overlap operators is to replace D_w in eq. (3) by alternative operators as proposed in Ref. 22.

2 Random Matrix Theory

Let us now start our discussion of finite volume physics with the example of a special technique called Random Matrix Theory (RMT). In many complex systems eigenvalues and their correlations play an important rôle. These eigenvalues may exhibit universal properties that can be described by RMT for many physical systems²⁴. Among the numerous application fields of RMT, also the low lying eigenvalues in the QCD spectrum are expected to be described by RMT (for a review, see Ref. 25). The theoretical background for this expectation is the fact that at zeroth order of chiral perturbation theory in the ϵ -regime, taking only the constant mode U_0 into account, the Lagrangians of chiral perturbation theory and the one of RMT are equivalent. Correspondingly, the LEC of chiral perturbation theory enter also the predictions of RMT, which in turn allows for their determination by confronting numerical data from lattice QCD simulations with the theoretical formulae from RMT.

Such a comparison of the predictions of RMT with numerical simulations is, however, difficult again, because also in this case the knowledge of the topological charge sectors

^bIn this approximation virtual quark anti-quark states are completely neglected. Although this seems to be a very crude approximation, it works surprisingly well in practice²³.

and an exact chiral symmetry are important. Both difficulties can be overcome elegantly with the use of operators solving the Ginsparg-Wilson relation. The limitation in this case will only be the computer time available, but with the machines available at NIC such a project becomes feasible, though with a rather limited statistics.

Another difficulty is that the finite volume cannot be arbitrarily small. Note that the Goldstone bosons of the chiral symmetry breaking pick up some mass if a small quark mass is switched on. The crucial point of chiral perturbation theory is that these quasi-Goldstone bosons represent the light mesons. Therefore, this effective low energy description can only work in the world of mesons as bound states. Hence the physical volume should — roughly speaking — be larger than the confinement scale. As we will see below, RMT can provide a quantitative answer to the question about the scale where the validity of chiral perturbation theory sets in.

In Figure 3 we show a result of such a computation²⁶. It addresses the cumulative probability distributions (see Ref. 27, Chapter 14) of the lowest (non-zero) Dirac eigenvalue λ_1 . For these distributions the predictions of RMT in various topological sectors (solid lines) are compared with the numerical data from our simulations using the overlap operator. We see that the data from the quenched simulations are well described by RMT.

Some remarks are in order. The first is that the data agree with the theoretical predictions only if the lattice corresponds to a physical volume of $V \gtrsim (1.2 \text{ fm})^4$. Going below this size, the predictions collapse. Hence a minimal box length of about 1.2 fm is necessary to be in the mesoscopic world where chiral perturbation and RMT work. The second remark is that from the probability distribution a value of the scalar condensate can be extracted and it is found to be consistent with earlier simulation results. The third remark concerns higher eigenvalues. Here the agreement is not as good as in the case of the leading non-zero eigenvalue. Generally the RMT predictions are confirmed up to some value of the dimensionless parameter $z = \lambda \Sigma V$. This threshold raises gradually if the volume increases, and it might be related to the so-called Thouless energy²⁵.

A last remark is of a more general nature: the prediction of the eigenvalue distribution by RMT for the lowest non-zero eigenvalue²⁸ in topological charge sector zero reads $P(\lambda) = \frac{z}{2} \exp(-\frac{1}{4}z^2)$. Hence, for simulations in this sector we expect to encounter quite frequently very small eigenvalues, which will contribute in quark propagators as $1/\lambda$. Now, from our comparison with RMT we know that the RMT predictions are well respected by the numerical data. Hence the small eigenvalues in topological charge sector zero *have to appear* in the simulations with a non-negligible probability. Clearly, they will give rise to substantial fluctuations in physical observables, providing exceptionally large contributions proportional to the inverse of the eigenvalue.

Of course, when the quark mass is chosen large enough it will act as an infrared regulator and therefore cut off the effects of these very small modes. In the ϵ -regime, however, we want to study the system at *small* quark masses. This leads to the problem of finding a window for simulations in the ϵ -regime: if the quark mass is too small, it cannot act as a regulator anymore and the small modes will spoil the statistical sample. When, on the other hand, the quark is chosen to be too large, we leave the ϵ -regime. The situation is clearly better when we choose a topologically non-trivial sector. Here RMT predicts an eigenvalue distribution that suppresses low eigenvalues substantially, rendering the simulations much safer. The problem discussed here is of a very general nature and does also apply to the case of dynamical fermions. Therefore, it has to be expected that these simulations become

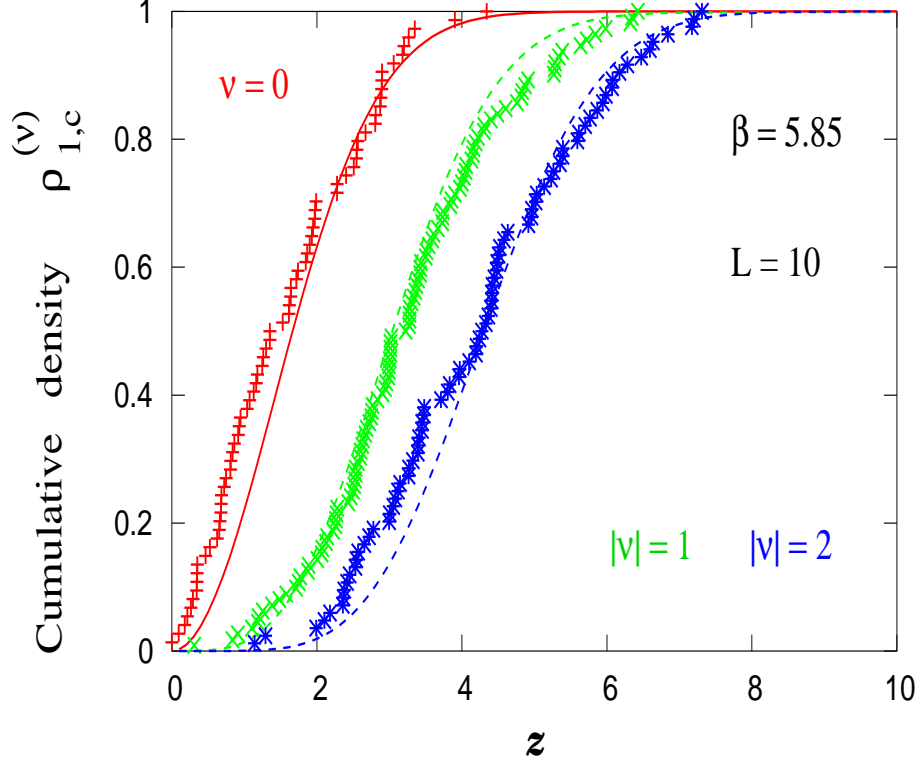


Figure 3. The cumulative probability distribution for the first non-zero eigenvalue in the topological sectors with charge $|\nu| = 0, 1, 2$, on a lattice of size $V = (1.23 \text{ fm})^4$.

very demanding and problematic if performed close to physical values of the quark masses. This is another motivation to understand the contact with chiral perturbation very well in order to let chiral perturbation theory do the job of computing observables at the physical point.

3 Meson Correlation Functions

In a previous NIC proceedings contribution²⁹ we reported about a test of spontaneous chiral symmetry breaking in QCD. For that study the evaluation of the zeroth order of chiral perturbation theory (involving only U_0) was necessary. In this follow-up project we also computed meson correlation functions in the ϵ -expansion regime for which the next order was known in the full theory⁷, but not in the quenched approximation. Therefore, new analytical computations were necessary for the quenched situation, a work that is published in Refs. 30,31. On the numerical side, the necessary propagators were computed using the overlap operator.

Restricting ourselves first to computations in topological charge sector zero, we found the correlation functions to be very noisy and with our limited statistics it was not possible

to extract a conclusive signal. We checked that this phenomenon can be understood from the eigenvalue distribution of RMT. Focusing on the contribution of the lowest eigenvalue alone (which is the largest contribution) and following Ref. 32 we estimated the statistics required to compute the scalar condensate from the correlation function based on the eigenvalue distribution of RMT. Indeed, we found that $O(10^4)$ configurations would be necessary to obtain reliable errors³³.

Therefore, we did not explore the topological charge sector zero any further and concentrated on topological charge sector one³⁴. Repeating the analysis from the theoretical eigenvalue distribution of RMT we found that with $O(100)$ configurations the errors tend to stabilize. From chiral perturbation theory we expect that in topological charge sectors $\pm\nu$ the correlation function of the axial current takes the form (in a volume $L^3 \times T$)

$$\begin{aligned} \langle A_\mu(0) A_\mu(t) \rangle_\nu &= \frac{F_\pi^2}{T} \left[1 + \frac{2m_q \Sigma_{|\nu|}(z_q) T^2}{F_\pi^2} \cdot h_1(\tau) \right], \\ h_1(\tau) &= \frac{1}{2} \left(\tau^2 - \tau + \frac{1}{6} \right), \quad \tau = \frac{t}{T}, \\ \Sigma_\nu(z_q) &= \Sigma \left(z_q \left[I_\nu(z_q) K_\nu(z_q) + I_{\nu+1}(z_q) K_{\nu-1}(z_q) \right] + \frac{\nu}{z_q} \right), \quad z_q = m_q \Sigma V. \end{aligned} \quad (7)$$

The first observation is that this correlation function does not show an exponential decay but a power law behavior, a clear reflection of the fact that the pion Compton wavelength is larger than the box size. In the axial correlation function there appear again the two LEC of the effective Lagrangian (1), F_π and Σ . In Figure 4 we show a fit of our data to the prediction of eq. (7). For our simulations we used a 12^4 lattice at $\beta = 6$ and worked in topological charge sector one. From the fit, the value of F_π can be determined quite reliably, whereas the value of Σ is rather insensitive and cannot be extracted. The situation here is somehow complementary to the fit of the spectrum to the RMT predictions that we discussed in Section 2.

Nevertheless, we see that chiral perturbation theory can be used to compute the LEC from meson correlation functions. The example of the axial current presented here can be extended to the scalar and the pseudo-scalar correlation functions (the vector correlation function is identically zero³¹), from which further LEC can be evaluated. However, in the formulae for those correlation functions additional parameters show up.

4 Conclusions

The somewhat unconventional ϵ -regime of chiral perturbation theory turns out to be an interesting, but also difficult region to be explored by means of numerical simulations. The parameters of the simulation have to be chosen with care: the topological charge must not be zero and the value of the quark mass has to be in a certain window in order to avoid problems with small eigenvalues on one side, and to avoid leaving the ϵ -expansion regime on the other side. If these precautions are taken care of, the LEC of the chiral Lagrangian can be computed from the numerical simulations with powerful consequences for future simulations in general.

The ϵ -regime served in this study as a kind of service setup to provide the LEC from “easy” to be done numerical simulations. By exploring the hypothetical world of

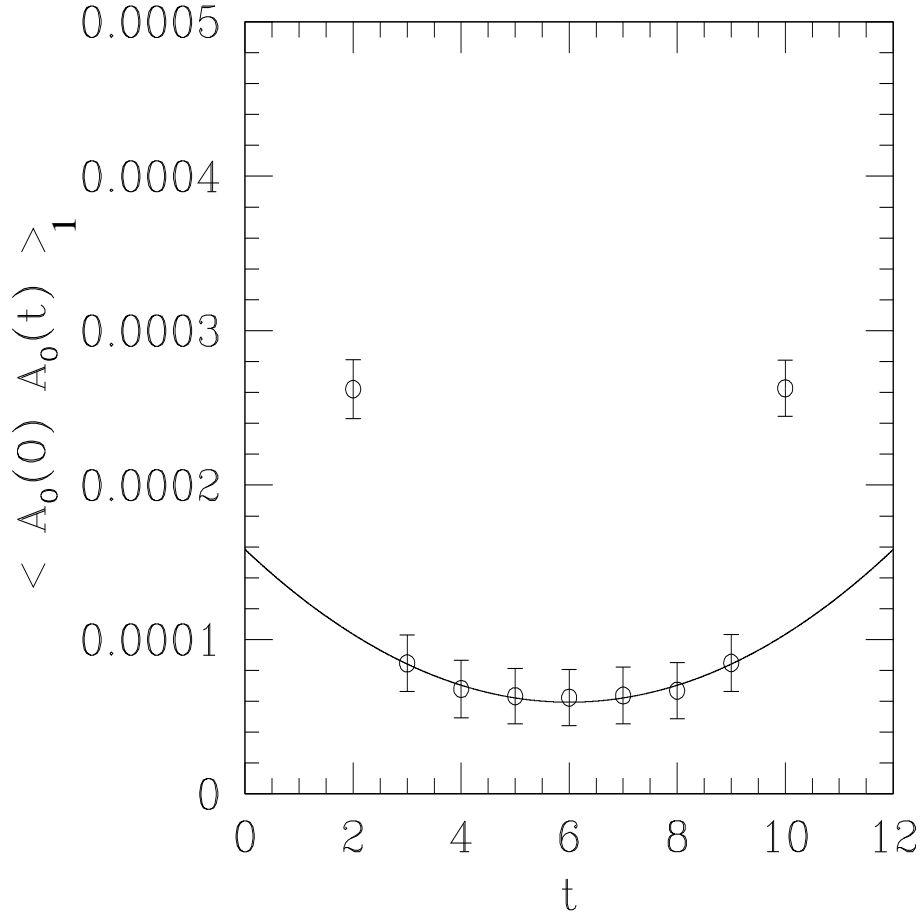


Figure 4. The axial correlation function on a 12^4 lattice at $\beta = 6$ in topological charge sector one. The solid line is a fit to the data using eq. (7).

quark masses that are much smaller than the physical ones — which can now be done in numerical simulations — the phenomenology of such a world could be tested. Possibly, in this way we could learn why the quarks have the masses they assume in nature. The results that will be obtained in the ϵ -regime might reveal some answers to such questions in the future and hence this regime may turn out to be not so unphysical after all.

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